# Fracture model for beryllium and other materials

Alek Zubelewicz (Theoretical Division) and Abigail Hunter (Computational Physics Division)

Los Alamos National Laboratory

Los Alamos, NM 87544

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# **Highlights**

The commonly used phenomenological constitutive models rely on a long-term trial-and-error approach, which led to the development of physically and numerically robust material descriptions. The phenomenology means that the models are "good" in the domain already verified by experiment. Quite often though, extrapolation of the models into the regimes not tested can be troublesome. For instance, these models don't generally account for specific plastic flow mechanisms such as plasticity and twinning. Beryllium seems to provide an example for such difficulties. In beryllium, we observe brittle-ductile transitions associated with complex fracture processes and the deformation mechanisms include plasticity and twinning. We break the phenomenology and construct a mechanisms-based model that captures deformation mechanisms due to plasticity and twinning and includes brittle and ductile fracture.

#### Introduction

Over several decades, Los Alamos National Laboratory (LANL) developed a set of excellent strength and fracture models for metals. While learning from the successes, the work has not stopped there because we believe that alternative modeling approaches should be pursued and validated, giving the chance for broadening the menu of LANL's modeling capabilities. In here, we introduce the mechanisms-based visco-plasticity model capable of replicating brittle and ductile fracture processes. The model is tested for beryllium showing excellent agreement with experimental data.

### Mechanisms-based approach

We adapt our earlier results [1] and construct the mechanisms-based visco-plasticity model with built-in fracture in the framework of a tensor representation theory [2]. First, physics-based insight dictates the selection of relevant mechanisms of inelastic deformation. Next, the magnitude of the flow due to plastic deformation and twinning is determined in terms of appropriate invariant strain rates. In our description, we enforce the principle of objectivity and, from there we derive equivalent (invariant) stresses compatible with plastic deformation and twinning. We emphasize that the invariant measures are derived and not assumed. In our model, the equivalent stresses are coupled with the equivalent strain rates. Also, we include the contribution of the dynamic overstress, which plays a role when the rate of the energy redistribution and dissipation is slower from the rate the energy is pumped into the material. Again, the formula for the overstress is derived and is based on thermodynamics considerations

[3]. Thus, the flow rules (mechanisms for plasticity and twinning) along with the rate dependent constitutive relations and, lastly, the dynamic overstress, complete the description of the inelastic behavior of beryllium. The visco-plasticity model has unique features, among which is the ability to capture the ductile-brittle transition, strain rate effects from quasi-static up to extreme conditions, shear localization at elevated temperature and cleavage at high strain rates and/or low temperatures.

#### **Brittle fracture**

A frequent assumption is that brittle fracture arises from a set of non-interacting penny-shaped micro-cracks randomly distributed in an otherwise homogeneous material [4]. Since the crack opening strain is collected from the individual micro-cracks, these descriptions are suitable for predicting the material's responses at early stages of the damage process. The cracks are characterized in terms of the crack surface area, while their orientations are defined in terms of stresses. One open issue in brittle materials is that these models predict an unlimited strength under bi-axial compression. This prediction seems unrealistic and, in fact, experimental observations gathered for various brittle materials provide arguments to the contrary [5, 6]. The penny-shape crack approach has been further extended in Ref. 7 but the previously mentioned concern of the non-interacting micro-cracks remains unsolved. In these constitutive models, fracture processes are built into the constitutive description by degrading either the material's strength or shear modulus.

Introduction of the micro-plane model [8] marks a significant progress in the understanding of the behavior of brittle/frictional materials. The model predicts the damage initiation and progressive growth and it captures fracture mechanisms occurring within a representative volume element (RVE) [9]. However, the introduction of RVE is a troublesome assumption, especially when considering an advanced stage of the post-critical behavior. The RVE homogenization technique fails at conditions where the cracks break up the volume. Also, the micro-plane model is quite complex and may present a challenge when applied to a large-scale numerical analysis. A relatively simpler model based on an analogous idea is proposed in Ref. 1. In this description, the fracture processes are monitored in terms of stress tractions along the dominant load directions and are acting on the crack opening displacements. As in many other cases, the fracture planes are co-rotational with principal stresses and, therefore, this model produces fracture that is stress-co-rotational, thus isotropic. Despite this deficiency, the model is strong in its simplicity and surprisingly good predictability.

In metals, damage processes are often assumed to follow the Gurson's ductile mechanism [10]. This mechanism accounts for the progression of a distributed damage due to the growth of voids in an already plastically deformed material. However, it has been long known that other ductile and brittle fracture mechanisms are present in various metals and, among them, in beryllium. The mechanisms can be sorted into two groups:

1 Ductile/brittle process zone due to either void growth and coalescence (ductile) or coalescence of micro-cracks (brittle). Both the processes follow the direction of the maximum tensile stress.

2 Shear localized zones caused by a shear dominant loading. As before, we may have a brittle fracture (cleavage) and there is temperature assisted shear localization.

The brittle and ductile fracture processes are included in the description of free energy. Following experimental observations, brittle fracture in beryllium includes mode I cracking (triggered by maximum tensile stress) and cleavage (mode II fracture) in compression. Also, we account for the brittle-ductile fracture transition in tension and shear. The transitions are observed below 200C and at high strain rates.

### Model calibration for beryllium

The proposed fracture model is calibrated using the existing experimental data at LANL. The model reproduces the material behavior (Figure 1) quite well. Yet in our assessment, the calibration cannot be considered complete. For instance, there is a coupling of the inelastic deformation due to twinning and plasticity but the interactions are not well understood. In here, we assume that some twins cannot be recovered in the presence of plastic deformation but we do not know the exact fraction of stored twins at various temperatures and strain rates. Also, the ductile-brittle transition appears to be not only temperature but also rate sensitive.

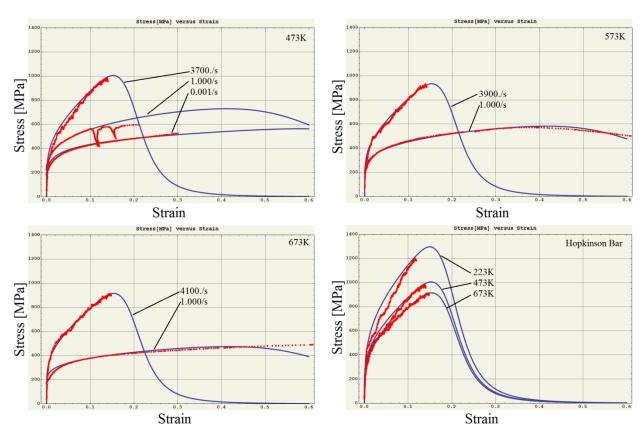


Fig. 1: Uniaxial stress-strain responses in beryllium at various temperatures and strain rates. The red lines depict the LANL experimental data, while the blue lines represent to the model predictions.

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